# THERMAL CONDUCTIVITY OF POROUS SILICON FILMS FROM FIRST PRINCIPLES

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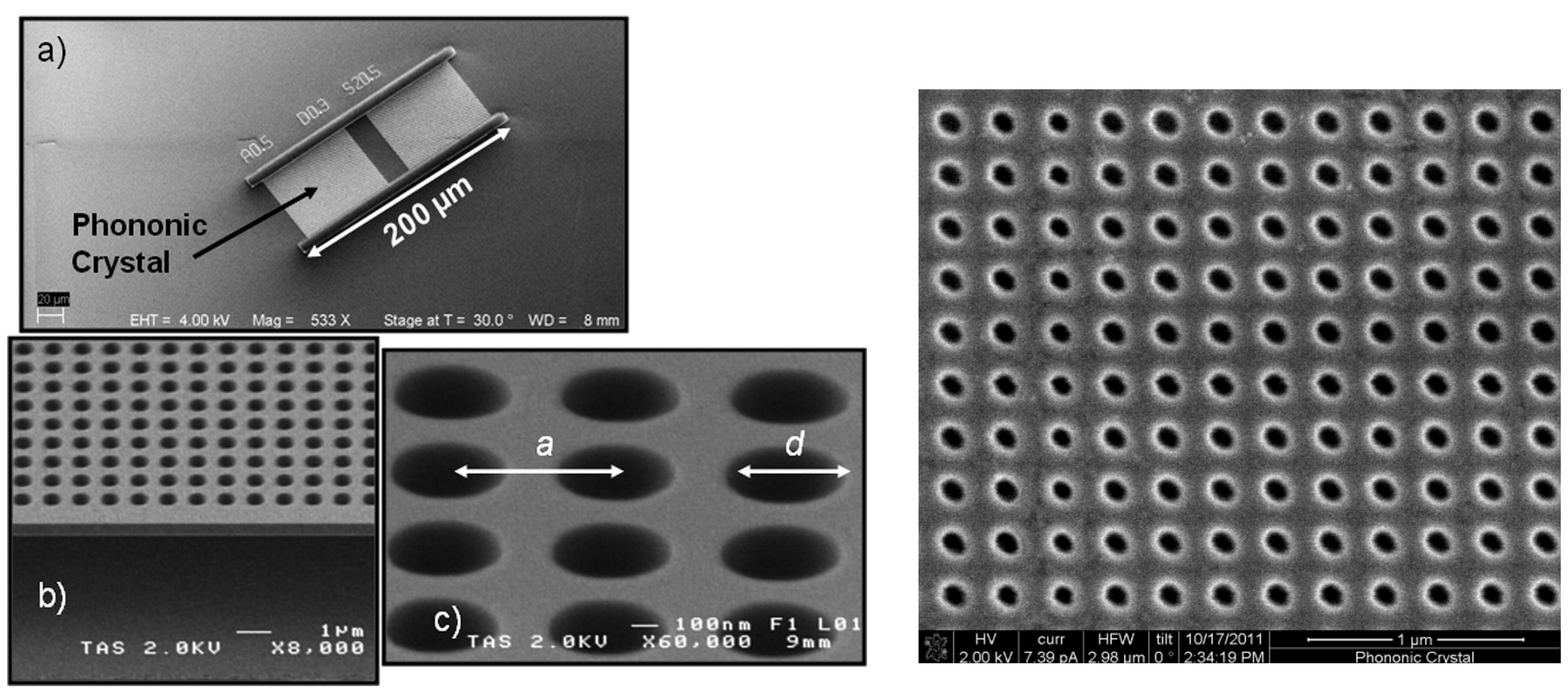
SUPPORT: AFOSR award FA95501010098

## Abstract

We predict the thermal conductivity of silicon thin films with a periodic arrangement of unfilled cylindrical pores and compare to experimental measurements. Lattice dynamics calculations, the Boltzmann transport equation, a Monte Carlo-based phonon-boundary scattering model, and finite element method calculations are used to identify the mechanisms of the thermal conductivity reduction.

## Introduction



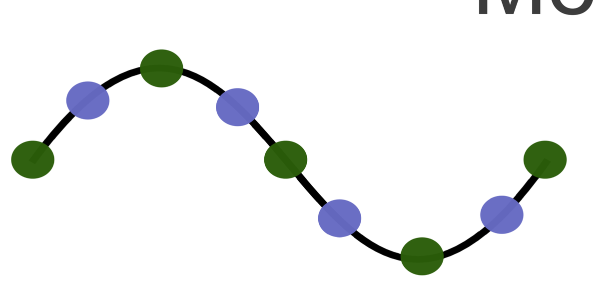

SEM images of silicon porous thin films studied by (left) Hopkins et al. [1] for cross-plane direction of heat flow, and (right) El-Kady et al. [2] for in-plane direction of heat flow.

**Film specifications**: thickness, *t*: 500 nm; pore size, *d*: 100-500 nm; pore separation, *a*: 100-800 nm; porosity, $\varphi = \pi d^2/4a^2$ : 0.05-0.40

### Computational Challenges

- **Molecular Dynamics:**
  Computationally expensive for system sizes greater than 100 nm.
- **Lattice Dynamics:**
  Cannot incorporate phonon scattering from boundaries.
- **Matthiessen Rule:**
  Ambiguity in the choice of system characteristic length.

## Methodology



Phonon (Lattice vibration)

- Phonon thermal conductivity,

$$k_n = \sum_i C_{ph,i} v_{g,n,i}^2 \frac{\Lambda_i}{|\mathbf{v}_{g,i}|}$$

$C_{ph}$: Volumetric specific heat

$\mathbf{v}_{g,i}$: Group velocity,

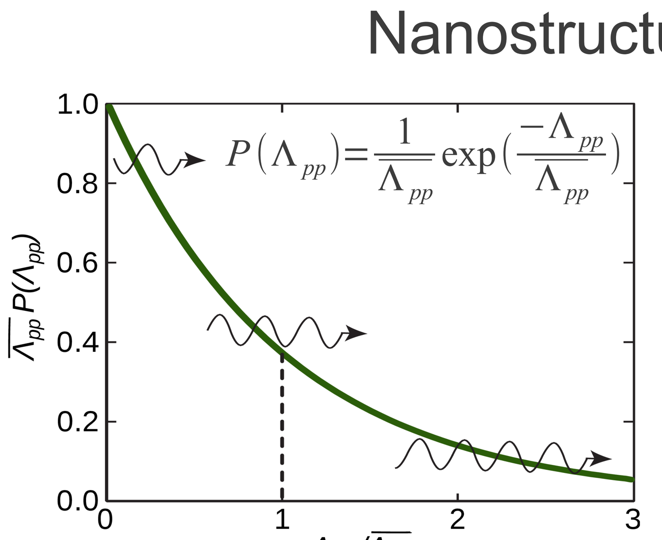
$$\mathbf{v}_{g,i} = \frac{d\omega_i}{d\boldsymbol{\kappa}}$$

$\Lambda_i$: Mean free path, i.e., average distance traveled by phonon before scattering.

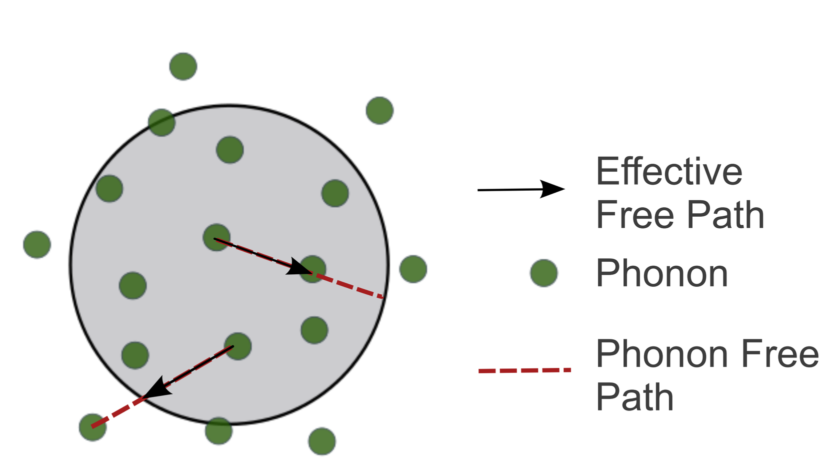
### Simulation Details

- Bulk phonon properties:
  Harmonic and anharmonic lattice dynamics calculations [3]
- Force constants:
  Density Functional Theory [4]
- Phonon boundary scattering:
  Monte Carlo based phonon free path sampling [5]
- Effect of material removal:
  Finite element method calculations
- Nanostructure boundaries:
  Diffuse

### Nanostructure Mean Free Path




Poisson distribution for phonon-phonon free path



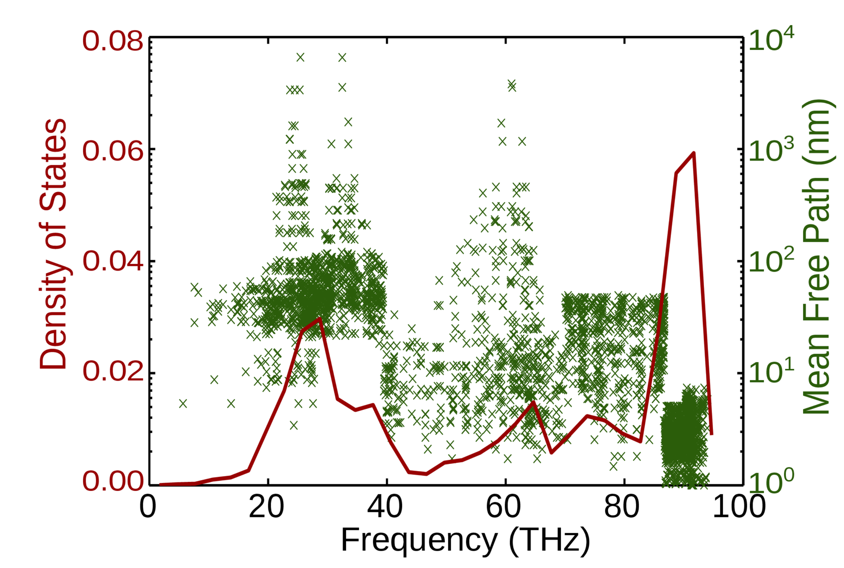

Uniform sampling of phonon initial position inside the nanostructure volume

$$\Lambda_{eff} = \min(\Lambda_{pp}, \Lambda_{pb})$$

$$\overline{\Lambda_{eff}} = \frac{\sum \Lambda_{eff}}{N}$$

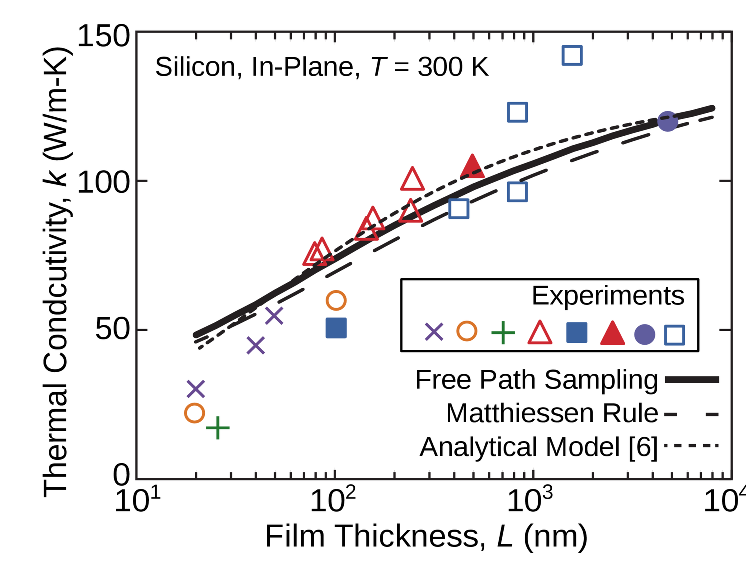
## Results

### Bulk Material



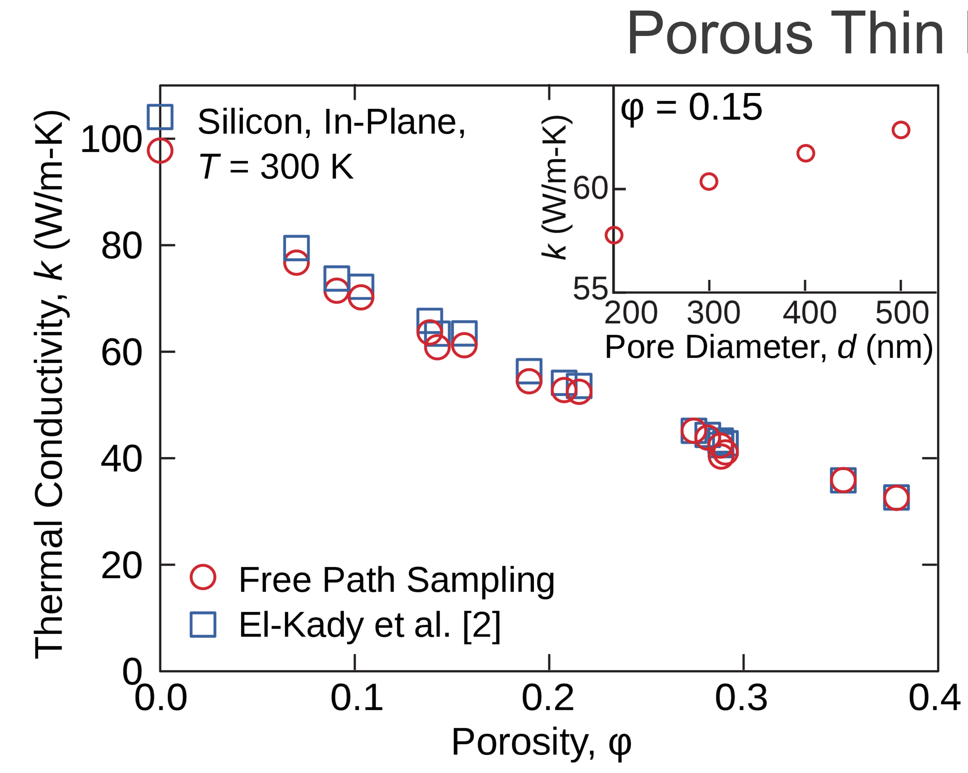

Dependence of phonon density of states and mean free path on frequency

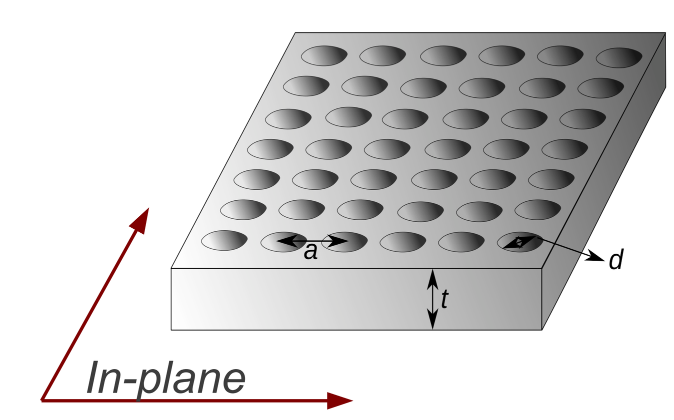
### Solid Thin Film



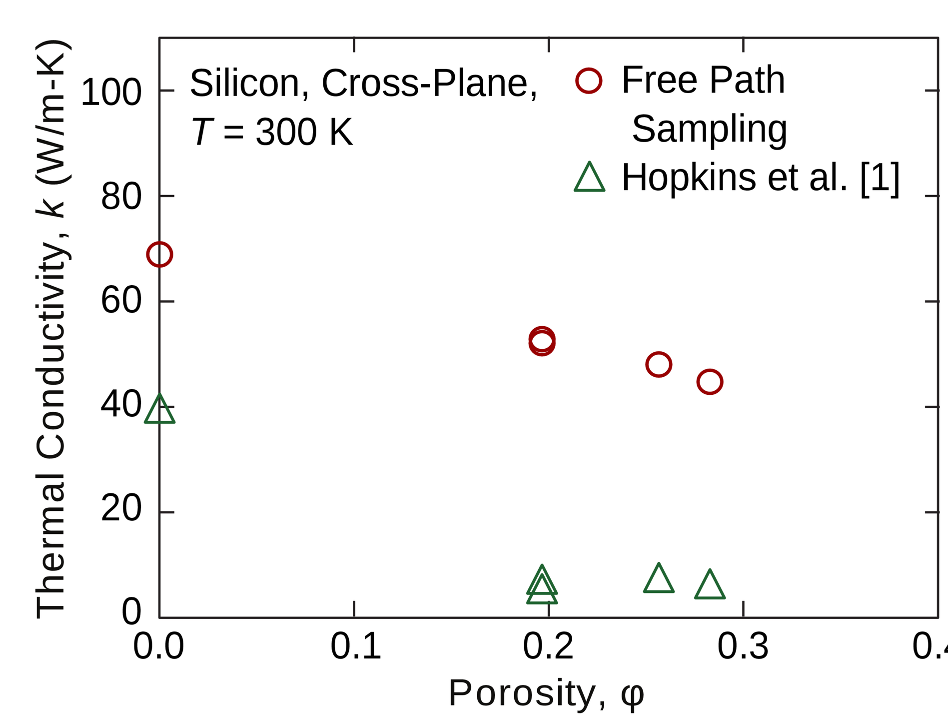

Thermal conductivity variation with film thickness in the in-plane direction.

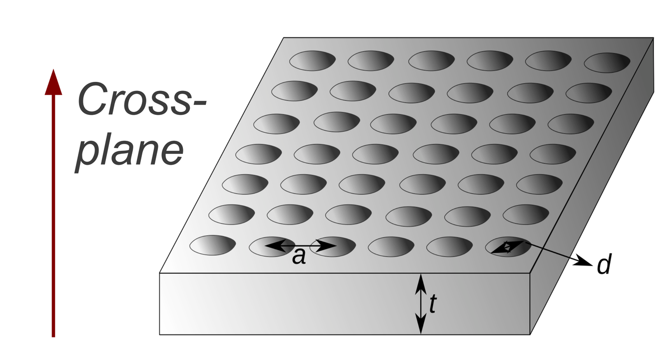
### Porous Thin Film



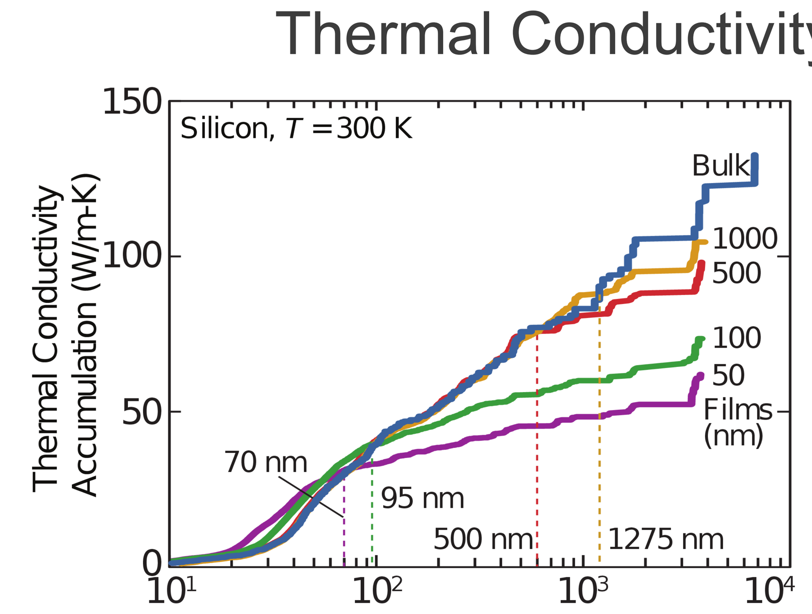

Thermal conductivity variation with porosity for heat flux in the in-plane direction



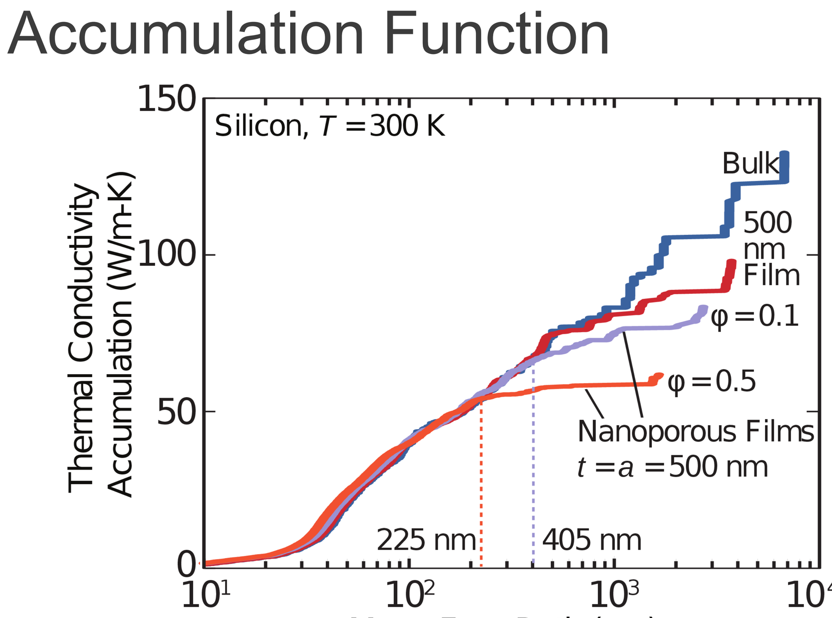




Thermal conductivity variation with porosity for heat flux in the cross-plane direction

### Thermal Conductivity Accumulation Function




Accumulation function for solid thin films




Accumulation function for porous thin films of porosity 0.1 and 0.5

## Conclusions

- In-plane thermal transport can be explained using free path model of phonons.
- Unexplained thermal conductivity for cross-plane direction of heat flow.
- Thermal conductivity accumulation function to define system thermal length scale.

## References and Acknowledgements

[1] Hopkins et al., Nano Letters **11**, 107 (2011).
[2] El-Kady et al., Progress Report SAND2012-0127.
[3] Turney et al., PRB **79**, 064301 (2009).
[4] Esfarjani et al., PRB 84, 085204 (2011).
[5] McGaughey and Jain, APL **100**, 061911 (2012).
[6] McGaughey et al., APL **99**, 131904 (2011).

Keivan Esfarjani for bulk phonon properties.